Thermodynamic Properties of Quinoxaline-1,4-Dioxide Derivatives – A Combined Experimental and Computational Study

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The melting points of the synthesized compounds, **1a**, **1b** and **1c,** were in excellent agreement with the published values reported in the literature (within 1 to 2 degrees of the published values).

1a: T_{mp} = 464 - 465 K (literature value, T_{mp} = 465 - 466 K taken from Haddadin, M. J.; Taha, M. U.; Jarrar, A. A.; Issidorides, C. H. Tetrahedron, 1976, 32, 719-724).

1b: T_{mp} = 406 - 407 K (literature value, T_{mp} = 405 - 406 K taken from Monge Vega, A.; Gil, M. J.; Fernandez-Alvarez, E. J. Heterocyclic Chem., 1984, 21, 1271-1275).

1c: T_{mp} = 432 - 434 K(literature value, T_{mp} = 432 - 433 K taken from Jarrar, A. A.; Fataftah, Z. A. Tetrahedron, 1984, 33, 2127-2129).

TABLE S1. Parameters of Clausius-Clapeyron equation and standard enthalpies of sublimation for **1a**.

Expt. No.	T/K	$\langle T \rangle$	a	b	-r	$\frac{\Delta_{cr}^{g} H_{m}^{\circ}(\langle T \rangle)}{kJ \cdot mol^{-1}}$	$\frac{\Delta_{cr}^{g} H_{m}^{\circ}(298.15K)}{kJ \cdot mol^{-1}}$
A	366.1 to 372.6	369.7	42.23 ± 1.67	14652 ± 617	0.9991	121.82	125.4
B	351.6 to 363.7	375.7	41.67 ± 0.28	14440 ± 99	0.9999	120.05	123.0
C	350.1 to 362.2	356.2	43.41 ± 0.24	15093 ± 87	0.9999	125.48	128.4
D	384.2 to 363.2	355.7	42.23 ± 0.37	14653 ± 133	0.9998	121.83	124.7
E	352.2 to 364.2	358.2	41.35 ± 0.44	14109 ± 158	0.9998	117.30	120.3

$\Delta_{cr}^{g} H_{m}^{\circ}(298.15K) = 124.4 \pm 2.7 \ kJ \cdot mol^{-1}$

TABLE S2. Parameters of Clausius-Clapeyron equation and standard enthalpies of sublimation for **1b** .

Expt. no.	T/K	$\langle T \rangle$	a	b	-r	$\frac{\Delta_{cr}^{g} H_{m}^{\circ}(\langle T \rangle)}{kJ \cdot mol^{-1}}$	$\frac{\Delta_{cr}^{g} H_{m}^{\circ}(298.15K)}{kJ \cdot mol^{-1}}$
A	368.3 to 380.2	374.1	43.67 ± 0.42	15712 ± 157	0.9998	130.63	134.4
B	360.6 to 375.6	368.1	42.23 ± 0.37	15193 ± 134	0.9998	126.31	126.8
C	362.1 to 374.1	368.1	43.04 ± 0.62	15489 ± 227	0.9997	128.78	132.3
D	364.2 to 376.1	370.1	44.23 ± 0.20	15896 ± 75	0.9999	132.16	135.8
E	365.6 to 377.6	371.6	44.02 ± 0.30	15779 ± 112	0.9999	131.19	134.9

$\Delta_{cr}^{g} H_{m}^{\circ}(298.15K) = 133.4 \pm 2.1 \ kJ \cdot mol^{-1}$

TABLE S3. Parameters of Clausius-Clapeyron equation and standard enthalpies of sublimation for **1c**.

Expt. no.	T/K	$\langle T \rangle$	a	b	-r	$\frac{\Delta_{cr}^{g} H_{m}^{\circ}(\langle T \rangle)}{kJ \cdot mol^{-1}}$	$\frac{\Delta_{cr}^{g} H_{m}^{\circ}(298.15K)}{kJ \cdot mol^{-1}}$
A	377.2 to 389.1	383.2	44.81 ± 0.43	17255 ± 163	0.9999	143.46	147.7
B	375.6 to 390.7	383.2	43.29 ± 1.02	16614 ± 389	0.9989	138.13	142.4
C	377.1 to 392.2	384.1	43.48 ± 0.62	16702 ± 238	0.9997	138.86	143.2
D	378.1 to 393.2	385.7	45.24 ± 0.42	17390 ± 163	0.9998	144.58	149.0
E	382.6 to 394.7	388.6	45.67 ± 0.12	17560 ± 49	0.9999	145.99	150.5

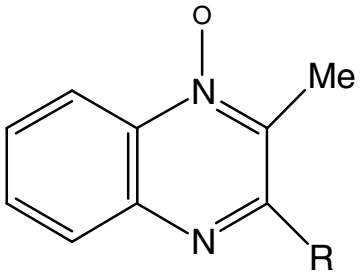
$\Delta_{cr}^{g} H_{m}^{\circ}(298.15K) = 146.6 \pm 3.2 \ kJ \cdot mol^{-1}$

TABLE S4. Calculated and experimental structures of **3** and **2a**.[a]

	2a			**3**	
	6-311+G(2d,2p) [b]	6-31G(d) [c]	EXPTL. [d]	6-311+G(2d,2p) [b]	6-31G(d) [c]
N1-C2	1.311	1.313	1.310	1.311	1.313
N1-C9	1.362	1.363	1.368	1.362	1.362
C2-C3	1.442	1.443	1.443	1.417	1.419
C10-C5	1.413	1.415	1.405	1.414	1.416
C5-C6	1.373	1.375	1.348	1.371	1.377
C6-C7	1.413	1.415	1.404	1.415	1.417
C9-C10	1.420	1.422	1.407	1.426	1.428
C2-R2	1.503	1.505	1.501	1.084	1.088
C8-H8	1.081	1.084	0.964	1.081	1.084
C7-H7	1.081	1.085	0.937	1.081	1.085
C9-N1-C2	118.1	117.9	117.7	116.6	116.3
N1-C2-C3	121.3	121.4	121.5	122.5	122.6
N1-C9-C10	120.6	120.7	120.8	120.9	121.0
C8-C9-N1	119.9	119.8	119.8	119.7	119.6
C8-C9-C10	119.5	119.4	119.3	119.4	119.3
C7-C8-C9	119.9	119.9	119.8	120.0	120.0
C8-C7-C6	120.6	120.6	120.8	120.7	119.9
N1-C2-R2	117.8	117.6	117.7	117.5	117.2
C9-C8-H8	118.2	118.1	119.1	118.1	117.8
C8-C7-H7	120.0	120.0	119.9	119.0	119.9

[a]Bond lengths in angstroms and bond angles in degrees. [b]This work. [c]Computed data taken from Matteo, A.; Valentin, M.; Giacometti, G.; Barone, V. *Chem. Phys. Lett*. 2001, 335, 427-434. [d]Crystallographic data taken from Wozniak, K.; Krygowski, T. M.; Kariuki, B.; Jones, W. *Acta Cryst*. 1990, 46, 1946-1947.

Scheme S1



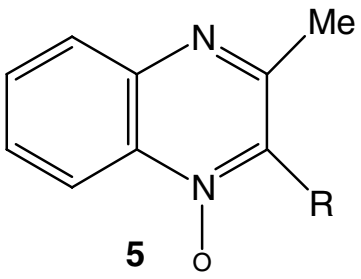
4

4a; R=Me

4b; R=C(O)OEt

4c; R=CH_2Ph

Scheme S2



5

5a; R=Me

5b; R=C(O)OEt

5c; R=CH_2Ph

Table S5. Optimized cartesian coordinates (Å), final energies (B3LYP/6-311+G(2d,2p), in Hartrees) and ZPEs (B3LYP/6-31G(d), in Hartrees). Please see text and schemes S1 and S2.

1a	0 imaginary frequencies Energy = -647.136313619 ZPE = 0.188449

N	-0.999898	0.000026	-1.061748
C	-1.001961	0.000027	0.332310
C	0.213855	-0.000025	1.033692
N	1.419655	-0.000064	0.334067
C	1.401268	0.000010	-1.022254
C	0.183470	-0.000007	-1.724789
C	0.215865	-0.000037	2.437057
C	-0.982116	0.000009	3.111733
C	-2.202032	0.000061	2.408022
C	-2.217773	0.000071	1.033205
O	2.529456	-0.000134	0.978212
C	2.754078	0.000092	-1.653723
C	0.052855	-0.000084	-3.211994
O	-2.113067	0.000065	-1.700036
H	-3.130824	0.000107	0.460003
H	-3.135311	0.000092	2.953062
H	-0.986691	0.000005	4.192502
H	1.169194	-0.000082	2.940428
H	2.703981	0.000770	-2.735234
H	3.317952	-0.870266	-1.315727
H	3.318271	0.869805	-1.314627
H	1.014157	-0.000446	-3.710071
H	-0.522321	0.870094	-3.530860
H	-0.522875	-0.869960	-3.530668

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1b	0 imaginary frequencies Energy = -875.075010948 ZPE = 0.231545

N	-1.865954	0.497083	-0.770840
C	-2.053570	0.268398	0.595281
C	-1.006214	-0.245927	1.379569
N	0.230658	-0.524322	0.792592
C	0.371086	-0.285561	-0.525994
C	-0.662484	0.214895	-1.322589
C	-1.198140	-0.480599	2.748421
C	-2.419962	-0.199282	3.313199
C	-3.469658	0.316880	2.529589
C	-3.294421	0.549700	1.185368
C	1.714873	-0.653656	-1.104656
O	2.623562	0.283086	-0.842791
C	3.987814	-0.010823	-1.258372
C	4.862359	1.126201	-0.782459
C	-0.529706	0.478030	-2.782938
O	1.898816	-1.656442	-1.743693
H	-4.075638	0.942256	0.554411
H	-4.424426	0.531967	2.988123
H	-2.575191	-0.377085	4.367805
H	-0.370461	-0.878124	3.313792
H	0.459300	0.217049	-3.144811
H	-0.737935	1.528254	-2.990648
H	-1.276951	-0.097081	-3.330671
H	4.272921	-0.964426	-0.817930
H	3.999542	-0.117821	-2.342058
H	5.895415	0.936023	-1.074409
H	4.551517	2.072675	-1.223371
H	4.823222	1.218207	0.301851
O	-2.824057	0.966818	-1.480162
O	1.188415	-1.004806	1.491537

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1c	0 imaginary frequencies Energy = -878.248173687 ZPE = 0.270484

C	-3.708539	0.567258	-0.771556
C	-2.416135	0.461672	-0.236565
C	-1.950858	-0.772141	0.244274
C	-2.779915	-1.903210	0.189625
C	-4.045268	-1.786599	-0.335986
C	-4.510756	-0.548594	-0.818406
N	-1.589709	1.584069	-0.183931
C	-0.344283	1.461922	0.333687
C	0.116920	0.229988	0.830710
N	-0.664497	-0.876841	0.776183
C	1.474001	0.058861	1.463089
C	2.602114	-0.194897	0.474270
C	2.551338	-1.277893	-0.408651
C	3.591996	-1.509492	-1.300179
C	4.701247	-0.668281	-1.322978
C	4.764138	0.405588	-0.443388
C	3.719671	0.638931	0.447255
O	-0.256578	-2.020744	1.200463
O	-2.015589	2.710028	-0.624891
C	0.463303	2.715922	0.320778
H	1.704012	0.943111	2.053749
H	-4.028682	1.532005	-1.130862
H	-5.507512	-0.473526	-1.229477
H	-4.687678	-2.654708	-0.379018
H	-2.389247	-2.834193	0.567184
H	-0.009282	3.473648	0.948390
H	1.480328	2.546526	0.651147
H	0.475234	3.127526	-0.688641
H	1.394234	-0.786397	2.145318
H	3.781317	1.476020	1.131568
H	5.622954	1.063075	-0.447817
H	5.509882	-0.851612	-2.017092
H	3.539295	-2.353294	-1.974875
H	1.703211	-1.948251	-0.378210

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2a	0 imaginary frequencies Energy = -496.751513328 ZPE = 0.179328

N	-0.958355	0.000000	-1.134130
C	-0.959917	0.000000	0.227804
C	0.261169	0.000000	0.951646
N	1.455172	0.000000	0.296513
C	1.439386	0.000000	-1.014617
C	0.199341	0.000000	-1.749661
C	0.232448	0.000000	2.364250
C	-0.971353	0.000000	3.024582
C	-2.186828	0.000000	2.304064
C	-2.185305	0.000000	0.931016
C	2.760558	0.000000	-1.731701
C	0.193105	0.000000	-3.252962
H	-3.102573	0.000000	0.359287
H	-3.124242	0.000000	2.843128
H	-0.994253	0.000000	4.105704
H	1.174330	0.000000	2.894468
H	3.566262	0.000000	-1.003135
H	2.864502	-0.876972	-2.373839
H	2.864502	0.876972	-2.373839
H	-0.833312	0.000000	-3.608584
H	0.705728	0.877075	-3.653200
H	0.705728	-0.877075	-3.653200

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2b	0 imaginary frequencies Energy = -724.694800126 ZPE = 0.222940

C	-3.623591	0.407315	0.162330
C	-2.213221	0.472455	0.084414
C	-1.470534	-0.725977	-0.101703
C	-2.148079	-1.964770	-0.202861
C	-3.516467	-1.998982	-0.123053
C	-4.256653	-0.806009	0.059552
N	-0.119513	-0.685526	-0.178511
C	0.467585	0.484310	-0.092466
C	-0.270449	1.707077	0.098368
N	-1.582226	1.670097	0.190931
C	1.967977	0.503728	-0.228743
O	2.588411	1.460622	-0.634475
C	0.382907	3.053087	0.233146
O	2.526807	-0.659287	0.119086
C	3.964418	-0.744802	-0.039636
C	4.391215	-2.123471	0.413354
H	-4.171841	1.328224	0.303101
H	-5.335535	-0.856998	0.118593
H	-4.040379	-2.941954	-0.199549
H	-1.558523	-2.860112	-0.341890
H	-0.375305	3.776489	0.521328
H	1.181745	3.039767	0.974757
H	0.840707	3.358985	-0.706683
H	4.207626	-0.562409	-1.085961
H	4.426875	0.044362	0.552591
H	5.471708	-2.225018	0.305273
H	4.134374	-2.288190	1.459302
H	3.911761	-2.897110	-0.185331

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2c	0 imaginary frequencies Energy = -727.863822448 ZPE = 0.261394

C	2.257775	-1.300662	-0.219878
C	2.410659	-0.160390	0.573064
C	3.624690	0.525658	0.525575
C	4.662897	0.087096	-0.291393
C	4.498894	-1.047436	-1.077828
C	3.292043	-1.740030	-1.038355
C	1.292763	0.300375	1.496888
C	-0.062485	0.398823	0.831942
N	-0.911019	-0.574677	1.059799
C	-2.132425	-0.517071	0.460714
C	-2.470397	0.574727	-0.380635
N	-1.581341	1.582400	-0.598755
C	-0.407148	1.511444	-0.019137
C	-3.074472	-1.547422	0.677908
C	-4.305673	-1.486808	0.073254
C	-4.641926	-0.400727	-0.766150
C	-3.744154	0.613501	-0.990991
C	0.558272	2.636980	-0.265958
H	1.567322	1.262357	1.931156
H	-3.980282	1.454204	-1.628059
H	-5.616988	-0.372102	-1.232861
H	-5.027899	-2.274515	0.238508
H	-2.795871	-2.367687	1.324520
H	1.488932	2.274372	-0.703835
H	0.102924	3.355366	-0.941791
H	0.818034	3.147240	0.664194
H	1.188065	-0.407972	2.319054
H	3.761499	1.410342	1.134743
H	5.596331	0.633202	-0.313619
H	5.302533	-1.389344	-1.715443
H	3.155840	-2.625171	-1.644957
H	1.325045	-1.847689	-0.191459

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3	0 imaginary frequencies Energy = -418.084546064 ZPE = 0.121582

N	-0.587167	0.000000	-1.764407
C	-0.589992	0.000000	-0.402953
C	0.631922	0.000000	0.332036
N	1.833710	0.000000	-0.307812
C	1.800438	0.000000	-1.618062
C	0.586003	0.000000	-2.348684
C	0.591466	0.000000	1.745783
C	-0.615702	0.000000	2.396130
C	-1.828086	0.000000	1.667127
C	-1.819764	0.000000	0.295835
H	-2.733382	0.000000	-0.281431
H	-2.768204	0.000000	2.201298
H	-0.646487	0.000000	3.476963
H	1.529860	0.000000	2.281843
H	2.748901	0.000000	-2.143594
H	0.605776	0.000000	-3.432820

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4a	0 imaginary frequencies Energy = -571.947316900 ZPE = 0.184265

N	-0.786032	0.000061	-0.973496
C	-0.787824	0.000036	0.426447
C	0.456187	0.000126	1.092994
N	1.641578	0.000213	0.426785
C	1.604033	0.000102	-0.889186
C	0.394849	-0.000042	-1.634649
C	0.447001	0.000125	2.507212
C	-0.741349	0.000030	3.194959
C	-1.971402	-0.000072	2.504276
C	-2.001277	-0.000070	1.129575
C	2.929535	0.000173	-1.604955
C	0.295309	-0.000283	-3.122340
O	-1.891036	-0.000260	-1.607561
H	-2.922737	-0.000125	0.569424
H	-2.898136	-0.000142	3.060610
H	-0.737648	0.000028	4.276241
H	1.400717	0.000196	3.014873
H	3.723659	0.000729	-0.864402
H	3.041808	-0.879524	-2.240544
H	3.041339	0.879267	-2.241439
H	1.275406	-0.000861	-3.586613
H	-0.267218	0.870629	-3.463538
H	-0.268086	-0.870782	-3.463134

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4b	0 imaginary frequencies Energy = -799.889686180 ZPE = 0.227551

N	-1.906664	0.262315	-0.700207
C	-1.989117	0.109340	0.688646
C	-0.806581	-0.181427	1.404740
N	0.395599	-0.315804	0.791749
C	0.418102	-0.184840	-0.516329
C	-0.708766	0.110132	-1.321480
C	-0.898216	-0.330427	2.808907
C	-2.107389	-0.192727	3.442156
C	-3.274938	0.098203	2.704171
C	-3.223814	0.249753	1.338686
C	1.755162	-0.439599	-1.173377
O	2.748790	0.168687	-0.524756
C	4.087602	-0.081973	-1.027350
C	5.051264	0.702897	-0.166425
C	-0.721912	0.316057	-2.796835
O	1.894881	-1.130812	-2.154534
H	-4.097128	0.472302	0.746819
H	-4.219791	0.202537	3.218684
H	-2.170453	-0.307650	4.515311
H	0.010078	-0.553217	3.349637
H	0.273782	0.244392	-3.215505
H	-1.167233	1.285476	-3.025035
H	-1.361017	-0.429729	-3.272772
H	4.273482	-1.154166	-0.981875
H	4.126718	0.221296	-2.072715
H	6.070857	0.533358	-0.513440
H	4.844387	1.771021	-0.221219
H	4.986542	0.391452	0.875198
O	-2.953813	0.542750	-1.365328

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4c	0 imaginary frequencies Energy = -803.059571410 ZPE = 0.265991

C	0.133186	-0.816888	-3.708096
C	0.122360	-0.815577	-2.305783
C	1.316868	-0.835319	-1.555327
C	2.541623	-0.855655	-2.262058
C	2.551540	-0.855221	-3.635014
C	1.342727	-0.836057	-4.361913
N	-1.093123	-0.795612	-1.611747
C	-1.086749	-0.788870	-0.257151
C	0.159840	-0.815017	0.423177
N	1.322552	-0.839239	-0.195632
C	0.209856	-0.811105	1.937115
C	-0.075305	0.538869	2.576531
C	0.540064	1.700771	2.104074
C	0.307081	2.926708	2.716893
C	-0.544497	3.012771	3.814493
C	-1.160172	1.862664	4.294695
C	-0.926588	0.637130	3.677637
O	-2.189234	-0.784335	-2.260522
C	-2.432768	-0.758797	0.382349
H	-0.481708	-1.551592	2.339820
H	-0.809307	-0.802506	-4.231735
H	1.367865	-0.837002	-5.442525
H	3.492837	-0.870517	-4.166885
H	3.454417	-0.871760	-1.684189
H	-3.016353	-1.627768	0.072604
H	-2.362024	-0.730941	1.463118
H	-2.989962	0.114282	0.039238
H	1.215634	-1.133665	2.206025
H	-1.408835	-0.253639	4.060897
H	-1.823546	1.916864	5.147278
H	-0.725953	3.966961	4.289688
H	0.792145	3.815845	2.337257
H	1.209400	1.643603	1.256231

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5a	0 imaginary frequencies Energy = -571.947316900 ZPE = 0.184265

N	-0.786032	0.000061	-0.973496
C	-0.787824	0.000036	0.426447
C	0.456187	0.000126	1.092994
N	1.641578	0.000213	0.426785
C	1.604033	0.000102	-0.889186
C	0.394849	-0.000042	-1.634649
C	0.447001	0.000125	2.507212
C	-0.741349	0.000030	3.194959
C	-1.971402	-0.000072	2.504276
C	-2.001277	-0.000070	1.129575
C	2.929535	0.000173	-1.604955
C	0.295309	-0.000283	-3.122340
O	-1.891036	-0.000260	-1.607561
H	-2.922737	-0.000125	0.569424
H	-2.898136	-0.000142	3.060610
H	-0.737648	0.000028	4.276241
H	1.400717	0.000196	3.014873
H	3.723659	0.000729	-0.864402
H	3.041808	-0.879524	-2.240544
H	3.041339	0.879267	-2.241439
H	1.275406	-0.000861	-3.586613
H	-0.267218	0.870629	-3.463538
H	-0.268086	-0.870782	-3.463134

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5b	0 imaginary frequencies Energy = -799.886067144 ZPE = 0.227200

N	-2.053068	0.603565	-0.850638
C	-2.218845	0.358829	0.478642
C	-1.197214	-0.181766	1.291695
N	0.039165	-0.469477	0.696001
C	0.185721	-0.210111	-0.617902
C	-0.883831	0.319329	-1.380451
C	-1.392263	-0.434283	2.656507
C	-2.613835	-0.141899	3.215683
C	-3.650696	0.399961	2.427991
C	-3.460639	0.645295	1.090260
C	1.513747	-0.577495	-1.219639
O	2.459236	0.306535	-0.900338
C	3.804370	0.003399	-1.363695
C	4.715188	1.103455	-0.868803
C	-0.688934	0.575237	-2.848716
O	1.664724	-1.534036	-1.936546
H	-4.241970	1.057772	0.468645
H	-4.605042	0.622629	2.884871
H	-2.781379	-0.329616	4.266757
H	-0.577474	-0.850861	3.227010
H	-1.596055	1.012814	-3.254396
H	0.144113	1.258596	-3.022666
H	-0.465185	-0.351429	-3.377571
H	4.082674	-0.972143	-0.968505
H	3.786706	-0.062570	-2.450569
H	5.736233	0.904071	-1.194998
H	4.412848	2.071933	-1.265793
H	4.706338	1.156277	0.218889
O	0.978532	-0.973837	1.384026

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5c	0 imaginary frequencies Energy = -803.058721249 ZPE = 0.266299

C	-0.325735	-0.823418	-3.861614
C	-0.326051	-0.816294	-2.447750
C	0.920572	-0.827535	-1.786915
C	2.129667	-0.843214	-2.497785
C	2.091692	-0.851052	-3.872294
C	0.858304	-0.841140	-4.556379
N	-1.507596	-0.796921	-1.775410
C	-1.461029	-0.795654	-0.460886
C	-0.247567	-0.810239	0.281528
N	0.930439	-0.817548	-0.385785
C	-0.183656	-0.837482	1.784378
C	-0.246221	0.533034	2.445022
C	0.706668	1.515033	2.156608
C	0.646127	2.758793	2.774113
C	-0.361725	3.042102	3.692154
C	-1.308723	2.070038	3.990670
C	-1.249697	0.825630	3.368830
O	2.051570	-0.814048	0.225228
C	-2.778160	-0.776955	0.266309
H	-1.006461	-1.445393	2.156387
H	-1.282721	-0.814481	-4.362931
H	0.848526	-0.846979	-5.637587
H	3.015336	-0.864125	-4.433584
H	3.054547	-0.848668	-1.943820
H	-2.840755	0.064077	0.956922
H	-3.578183	-0.700585	-0.463868
H	-2.923351	-1.689303	0.848366
H	0.747892	-1.330518	2.060567
H	-1.990100	0.073415	3.610631
H	-2.093859	2.276764	4.705379
H	-0.405248	4.010346	4.171739
H	1.391710	3.507255	2.541827
H	1.503410	1.291965	1.460575

Table S6. Geometries (Å) and enthalpies (Hartree) of CH_2NH and CH_2NCH_3 computed at the G3 level of theory.

CH_2NH	0 imaginary frequencies G3 Enthalpy at T = 298.15 K: -94.550993 C -0.501279 0.000000 0.316017 H -0.531646 0.000000 1.404756 N 0.641942 0.000000 -0.261128 H -1.470394 0.000000 -0.193090 H 0.516118 0.000000 -1.279873
CH_2NCH_3	0 imaginary frequencies G3 Enthalpy at T = 298.15 K: -133.815892 C 0.503223 -0.125981 -1.074486 N 0.501949 0.213459 0.156129 H 1.408494 0.019048 -1.661505 H -0.362406 -0.562419 -1.591339 C -0.737995 -0.005850 0.885609 H -0.532466 -0.664663 1.733222 H -1.080372 0.951138 1.287690 H -1.538260 -0.446329 0.272289